

=> b reg  
 FILE 'REGISTRY' ENTERED AT 13:04:38 ON 04 APR 2008  
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STRUCTURE FILE UPDATES: 3 APR 2008 HIGHEST RN 1012038-13-9  
 DICTIONARY FILE UPDATES: 3 APR 2008 HIGHEST RN 1012038-13-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

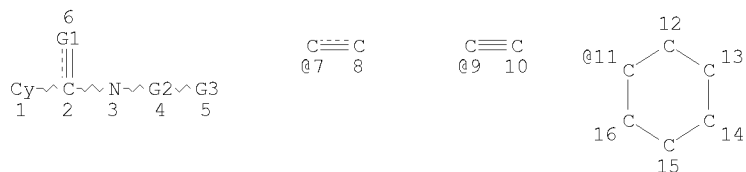
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
 predicted properties as well as tags indicating availability of  
 experimental property data in the original document. For information  
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d que sta l17  
 L11 STR



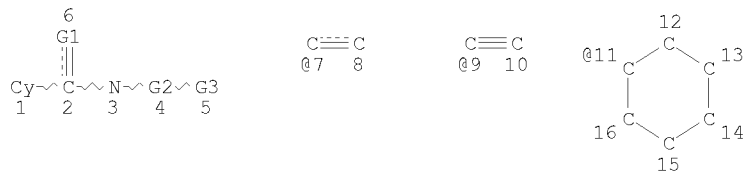
VAR G1=O/S  
 REP G2=(1-3) C  
 VAR G3=7/9/11  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE  
 L13 SCR 1011 OR 1012 OR 1013 OR 1019  
 L15 SCR 1840  
 L17 17940 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L15

100.0% PROCESSED 696595 ITERATIONS 17940 ANSWERS  
 SEARCH TIME: 00.00.13

=> d que sta l23  
 L11 STR

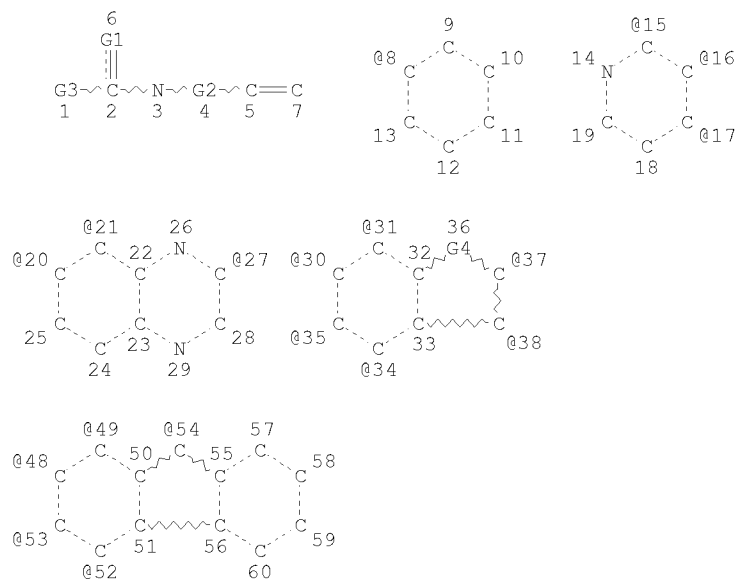


VAR G1=O/S  
 REP G2=(1-3) C  
 VAR G3=7/9/11

NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE  
 L13 SCR 1011 OR 1012 OR 1013 OR 1019  
 L15 SCR 1840  
 L17 17940 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L15  
 L20 STR



VAR G1=O/S  
 REP G2=(1-3) C  
 VAR G3=8/15/16/17/27/20/21/37/38/30/31/34/35/54/48/49/52/53  
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NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

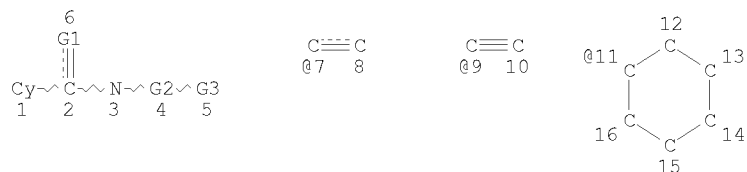
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 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 51

STEREO ATTRIBUTES: NONE  
 L23 8285 SEA FILE=REGISTRY SUB=L17 SSS FUL L20

100.0% PROCESSED 13960 ITERATIONS  
 SEARCH TIME: 00.00.01

8285 ANSWERS

=> d que sta l30  
 L11 STR



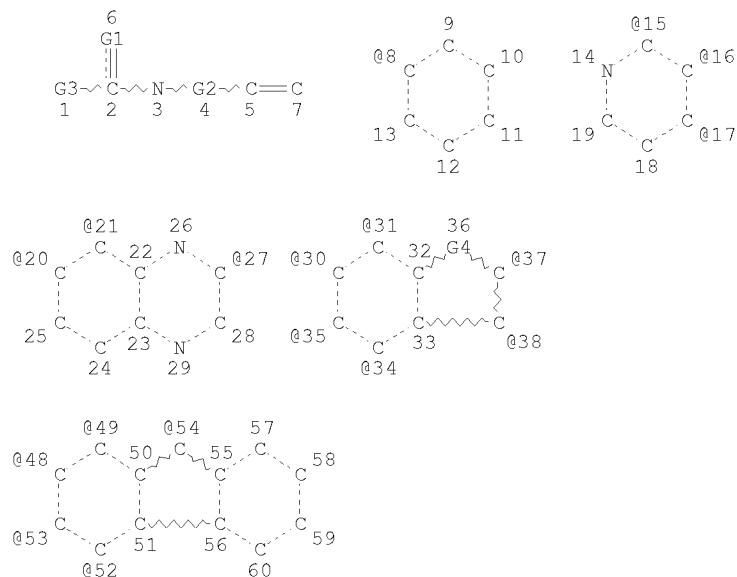
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 REP G2=(1-3) C

VAR G3=7/9/11  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L13 SCR 1011 OR 1012 OR 1013 OR 1019  
 L15 SCR 1840  
 L17 17940 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L15  
 L20 STR



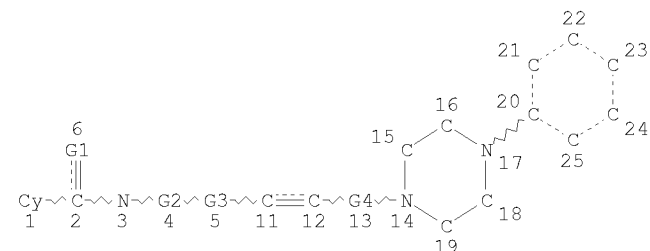
VAR G1=O/S  
 REP G2=(1-3) C  
 VAR G3=8/15/16/17/27/20/21/37/38/30/31/34/35/54/48/49/52/53  
 VAR G4=O/S  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 51

STEREO ATTRIBUTES: NONE

L23 8285 SEA FILE=REGISTRY SUB=L17 SSS FUL L20  
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 L25 STR

C≡C C≡C  
 @7 @8 @9 @10



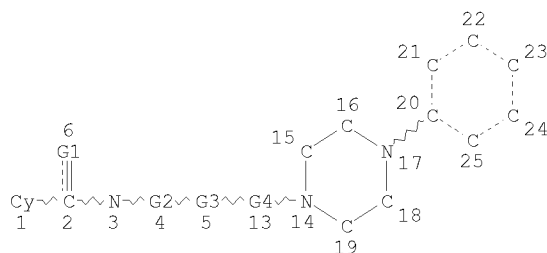
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REP G2=(1-3) C  
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 REP G4=(0-3) C  
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE  
 L26 STR

C≡C C≡C  
 @7 @8 @9 @10



VAR G1=O/S  
 REP G2=(1-3) C  
 VAR G3=7-4 8-13/9-4 10-13/CB  
 REP G4=(0-3) C  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE  
 L30 13 SEA FILE=REGISTRY SUB=L24 SSS FUL (L25 OR L26)

100.0% PROCESSED 267 ITERATIONS 13 ANSWERS  
 SEARCH TIME: 00.00.01

=> b hcap  
 FILE 'HCAPLUS' ENTERED AT 13:04:51 ON 04 APR 2008  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 4 Apr 2008 VOL 148 ISS 15  
 FILE LAST UPDATED: 3 Apr 2008 (20080403/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

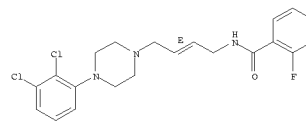
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d bib abs hitrn fhitrn 145 tot

145 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS ON STN (Continued)  
 AN 2005:31512 HCAPLUS  
 DN 142:190237  
 TI Novel Heterocyclic Trans Olefin Analogues of N-[4-[(2,3-Dichlorophenyl)piperazin-1-yl]butyl]arylcaboxamides as Selective Probes with High Affinity for the Dopamine D3 Receptor  
 AU Grundt, Peter; Carlson, Erin E.; Cao, Jianjing; Bennett, Christina J.; McIlveen, Elizabeth; Taylor, Michelle; Luedtke, Robert R.; Newman, Amy Hauck  
 CS Medicinal Chemistry Section National Institute on Drug Abuse-Intramural Research Program, National Institutes of Health, Baltimore, MD, 21224, USA  
 SO Journal of Medicinal Chemistry (2005), 48(3), 839-848  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DI Journal  
 LA English  
 OS CASREACT 142:190237  
 AB Dopamine D3 receptor subtypes have been hypothesized to play a pivotal role in modulating the reinforcing and drug-seeking effects induced by cocaine. However, definitive pharmacol. investigations have been hampered by the lack of highly D3 receptor selective compds. that can be used in vivo. To address this problem, the potent and D3-receptor-selective antagonist MGB 2904 (1, 9H-fluorene-2-carboxylic acid 4-[(2,3-dichlorophenyl)-piperazin-1-yl]-butyl]-amide, K<sub>i</sub> (hD3) = 2.0 nM, K<sub>i</sub> (hD2L) = 112 nM, D2/D3 selectivity ratio of 56) was chosen as a lead structure for chemical modification in an attempt to reduce its high lipophilicity (c log D = 6.94) while optimizing D3 receptor binding affinity and D2/D3 selectivity. A series of >30 novel analogs were synthesized, and their binding affinities were evaluated in competition binding assays in HEK 293 cells transfected with either D2L, D3, or D4 human dopamine receptors using the high affinity, selective D2-like receptor antagonist 125I-IABN. Structural diversity in the aryl amide end of the mol. was found to have a major influence on (sub)nanomolar D3 receptor affinity and D2/D3 selectivity, which was optimized using a more rigid trans-butenyl linker between the aryl amide and the piperazine. Several analogs demonstrated superior D3 receptor binding affinities and selectivities as compared to the parent ligand. Compound 29 (N-[4-[(2,3-dichlorophenyl)-piperazin-1-yl]-trans-but-2-enyl]-4-pyridine-2-yl-benzamide) displayed the most promising pharmacol. profile (K<sub>i</sub> (hD3) = 0.7 nM, K<sub>i</sub> (hD2L) = 93.3 nM, D2/D3 selectivity ratio of 133). In addition, this ligand inhibited quinpirole stimulation of mitogenesis at human dopamine D3 receptors transfected into Chinese hamster ovary (CHO) cells, with an EC<sub>50</sub> value of 3.0 nM. Compound 29 was a nearly 5 times more potent antagonist at the D3 receptor than 1 (EC<sub>50</sub> = 14.4 nM). Moreover, a decrease in c log D value of .apprx.2 orders of magnitude was determined for this novel D3-receptor-prefering ligand, compared to 1. In summary, chemical modification of 1 has resulted in compds. with high affinity and selectivity for D3 receptors. The most promising candidate, compound 29, is currently being evaluated in animal models of cocaine abuse and will provide an important tool with which to elucidate the role of D3 receptors in drug reinforcement in vivo.  
 IT 675599-29-8P 675599-30-1P 675599-31-2P  
 675599-32-3P 675599-34-5P 675599-35-6P  
 675599-36-7P 675599-38-9P 675599-39-0P  
 675599-45-8P 675599-46-9P 675599-47-0P  
 675599-48-1P 675599-49-2P 675599-52-7P  
 675599-53-8P 675599-54-9P 675599-55-0P  
 675599-56-1P 675599-58-3P 675599-59-4P  
 675599-61-8P 675599-62-9P 675599-64-1P  
 RL PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (N-[4-[(2,3-Dichlorophenyl)piperazin-1-yl]butyl]arylcaboxamide derivs.: preparation and affinity for D3 receptor)  
 IT 675599-29-8P  
 RL PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (N-[4-[(2,3-Dichlorophenyl)piperazin-1-yl]butyl]arylcaboxamide derivs.: preparation and affinity for D3 receptor)  
 RN 675599-29-8 HCAPLUS

145 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS ON STN (Continued)  
 CN Benzamide, N-[(2E)-4-[(4-(2,3-dichlorophenyl)-1-piperazinyl)-2-butenyl]-2-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● 2 HCl

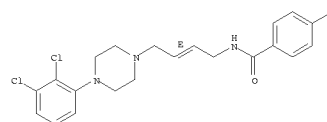
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

145 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS ON STN (Continued)  
 AN 2004:252605 HCAPLUS  
 DN 140:287411  
 TI Preparation of structurally rigid arylpiperazines as dopamine D3 receptor selective ligands  
 AU Newman, Amy; Grundt, Peter; Luedtke, Robert R.  
 PA United States Department of Health and Human Services, USA  
 SO PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DI Patent  
 LA English  
 FAN.CNT 1  

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO-2004024878	A2	20040325	2003WO-US0028895	20030915
WO-2004024878	A3	20040701		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BG, BR, BY, BE, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SH, SI, TJ, TN, TR, TT, TZ, UA, UG, US, VC, VE, VN, YU, ZA, ZM, ZW			
PW:	GH, GM, KE, LS, MW, ME, SD, SL, SZ, TE, UG, ZM, ZW, AM, AZ, BY, KG, KE, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA-----2498936	A1	20040325	2003CA-002498936	20030915
AU-2003267201	A1	20040430	2003AU-00267201	20030915
US-20060106030	A1	20060518	2005US-000527594	20051213
PRAI 2002US-00410715P	P	20020914		
2002WO-US0028895	W	20030915		
OS MAPPAT 140:287411				
GI				

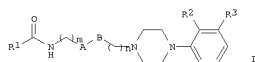
145 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS ON STN (Continued)  
 IT 675599-27-6P  
 RL PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of structurally rigid arylpiperazines as dopamine D3 receptor selective ligands)  
 RN 675599-27-6 HCAPLUS  
 CN Benzamide, N-[(2E)-4-[(4-(2,3-dichlorophenyl)-1-piperazinyl)-2-butenyl]-4-iodo-, ethanediolate (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 675599-26-5  
 CMF C21 H22 Cl2 I N3 O

Double bond geometry as shown.



CM 2

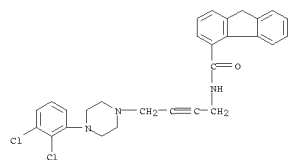
CRN 144-62-7  
 CMF C2 H2 O4



AB Title compds. [I; A = CH:CH, C.tplbond.C, cyclohexylene; B = null, CH:CH; R1 = (substituted) Ph, heteroaryl; R2 = H, halo, alkoxy; R3 = H, halo], were prepared. Thus, carbonylidimidazole was stirred 1 h with 4-hydroxybenzoic acid in pyridine; 4-[(2,3-dichlorophenyl)piperazin-1-yl]but-2-enylamine (preparation given) in CHCl3 was added followed by stirring overnight to give 514 N-[4-[(2,3-dichlorophenyl)piperazin-1-yl]but-2-enyl]-4-hydroxybenzamide (PG01015). PG01015 bound to cloned human D3 receptors in HEK cells with 34-fold greater affinity than to D2 receptors.  
 IT 675599-27-6P 675599-28-7P  
 RL PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of structurally rigid arylpiperazines as dopamine D3 receptor selective ligands)  
 IT 675599-29-8 675599-30-1 675599-31-2  
 675599-32-3 675599-34-5 675599-35-6  
 675599-36-7 675599-38-9 675599-39-0  
 675599-41-4 675599-43-6 675599-45-8  
 675599-46-9 675599-47-0 675599-48-1  
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 RL PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (preparation of structurally rigid arylpiperazines as dopamine D3 receptor selective ligands)

=> d bib abs hitstr l44 tot

L44 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on SIN  
 AN 2003:442759 HCAPLUS  
 DN 139:230723  
 TI N-[4-[4-(2,3-dichlorophenyl)piperazin-1-yl]butyl, butenyl and  
 butynylarylcarboxamides as novel dopamine D3 receptor antagonists  
 AU Newman, Amy Hauck; Cao, Jianjing; Bennett, Christina J.; Robarge, Michael  
 J.; Freeman, Rebekah A.; Luedtke, Robert R.  
 CS Medicinal Chemistry Section, Intramural Research Program, National  
 Institute on Drug Abuse, Baltimore, MD, 21224, USA  
 SO Bioorganic & Medicinal Chemistry Letters (2003), 13(13), 2179-2183  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 AS CASREACT 139:230723  
 The dopamine D3 receptor subtype has been targeted as a potential  
 neurochem. modulator of the behavioral actions of psychomotor stimulants,  
 such as cocaine. Previous synthetic studies provided structural  
 requirements for high affinity binding to D3 receptors which included a  
 2,3-dichloro-phenylpiperazine linked to an arylamido function via a Bu  
 chain. To reduce lipophilicity of these agents and further investigate  
 optimal conformation, a second series of 19 novel ligands was designed  
 that included heteroatom, substitution and unsatd. alkyl linkers. These  
 compds. were synthesized and evaluated for binding at rat D3 and D2  
 receptors stably expressed in Sf9 cells. D3 binding affinities ranged  
 from Ki = 0.6-1080 nM, with a broad range of D3/D2 selectivities (2-97).  
 The discovery of potent, selective and bioavailable D3 receptor ligands  
 will provide essential mol. probes to elucidate the role D3 receptors play  
 in the psychomotor stimulant and reinforcing effects of cocaine.  
 IT 595584-53-SP 595584-55-7P 595584-57-9P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 SO (preparation of [(dichlorophenyl)piperazinyl]but(en)(yn)ylarylcarboxamides  
 as novel dopamine D3 receptor antagonists)  
 RN 595584-53-5 HCAPLUS  
 CN 9H-Fluorene-4-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]-2-  
 butynyl]-, ethanedioate, hydrate (4:1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 595584-52-4  
 CMF C28 H25 Cl2 N3 O



CM 2  
 CRN 7732-18-5  
 CMF H2 O

H2O

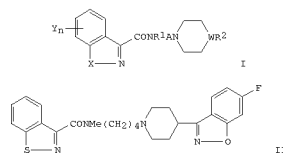
L44 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on SIN (Continued)  
 RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT



L44 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on SIN (Continued)  
 CM 3  
 CRN 144-62-7  
 CMF C2 H2 O4  
  
 RN 595584-55-7 HCAPLUS  
 CN 9H-Fluorene-2-carboxamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]-2-  
 butynyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 595584-54-6  
 CMF C28 H25 Cl2 N3 O  
  
 CM 2  
 CRN 144-62-7  
 CMF C2 H2 O4  
  
 RN 595584-57-9 HCAPLUS  
 CN Benamide, N-[4-[4-(2,3-dichlorophenyl)-1-piperazinyl]-2-butynyl]-,  
 ethanedioate (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 595584-56-8  
 CMF C21 H21 Cl2 N3 O  
  
 CM 2  
 CRN 144-62-7  
 CMF C2 H2 O4

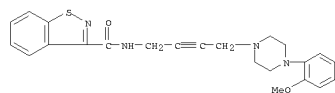
L44 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on SIN  
 AN 1993:80954 HCAPLUS  
 DN 118:80954  
 TI Preparation of N-[4-[(hetero)aryl]piperazinoalkyl]benzothiazole-3-  
 carboxamides and analogs as antipsychotics  
 IN Hrib, Nicholas J.; Jurcak, John G.  
 PA Hoechst-Roussel Pharmaceuticals Inc., USA  
 SO U.S., 14 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1  

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US-----5143923	A	19920901	1991US-000693168	19910429
CA-----2067404	A1	19921030	1992CA-002067404	19920408
CA-----2067404	C	20030819		
EP-----511610	A1	19921104	1992EP-000107138	19920427
EP-----511610	B1	19960911		
R: A2, B6, CH, DE, DK, ES, FR, GB, GR, IT, IL, LU, NL, PT, SE				
IL-----101700	A	19951127	1992IL-000101700	19920427
PL-----168090	B1	19960131	1992PL-000294358	19920427
PL-----168870	B1	19960430	1992PL-000309056	19920427
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NO-----180488	B	19970120		
NO-----180488	C	19970430		
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AU-----644054	B2	19931202		
JP-----0512472	A	19930528	1992JP-000108229	19920428
RU-----2039057	C1	19950709	1992RU-005011480	19920428
CZ-----282764	B6	19971015	1992CZ-000001298	19920428
EP-----215345	B1	19990816	1992EP-000007140	19920428
HU-----62889	A2	19930628	1992HU-000001414	19920429
HU-----214032	B	19971229		
US-----5225412	A	19930706	1992US-000899518	19920616
US-----5143923	B1	19931102	1992US-090002891	19921116
PRAI 1991US-000693168	A	19910429		
OS MARPAT 118:80954				
GI				



AB Title compds. [I: A = alkylene, CHR4ZCHR4; R1 = H, alkyl; R2 = alkyl,  
 (substituted) Ph, -PhCH2, -Br, -pyrimidyl, -benzisoxazol-3-yl, etc.; W =  
 N, CH; X = O, S; Y = H, alkyl, alkoxy, OH, halo, CF3; Z = CH:CH,  
 C:tpbond; C: n = 1, 2] were prepared. Thus, N-methyl-N-(4-bromobutyl)-1,2-  
 benzisothiazole-3-carboxamide was condensed with 4-(6-fluoro-1,2-  
 benzisoxazol-3-yl)piperidine to give title compound II, which had ED50 of  
 1.5 mg/kg i.p. against apomorphine-induced climbing in mice.  
 IT 145759-36-OP 145759-37-1P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
 BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of, as antipsychotic)  
 RN 145759-36-0 HCAPLUS  
 CN 1,2-Benzisothiazole-3-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-

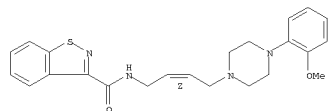
L44 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on SIN (Continued)  
 piperazinyl]-2-butyryl]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 145759-37-1 HCAPLUS  
 CN 1,2-Benzisothiazole-3-carboxamide, N-[4-[(2-methoxyphenyl)-1-piperazinyl]-2-butenyl]-, dihydrochloride, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● 2 HCl



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CA INDEXING COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

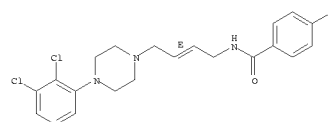
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CA INDEXING COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitrn fhitstr 142 1
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L42 ANSWER 1 OF 3 USPATFULL on STN  
AN 2006125885 USPATFULL  
TI Structurally rigid dopamine d3 receptor selective ligands and process  
for making them  
IN Newman, Amy, Phoenix, MD, UNITED STATES  
Grundt, Peter, Baltimore, MD, UNITED STATES  
Luedtke, Robert R., Fort Worth, TX, UNITED STATES  
PA Gov't of the USA as represented by The Secretary of the Department of  
Health and Human Services, Rockville, MD, UNITED STATES, 20852 (U.S.  
corporation)  
PI US-20060106030 A1 20060518  
AI 2003US-000527594 A1 20030915 (10)  
2003WO-US0028895 20030915  
20051213 PCT 371 date  
PRAI 2002US-000410715P 20020914 (60)  
DT Utility  
FS APPLICATION  
LRBP Birch, Stewart, Kolasch & Birch, LLP, 8110 Gatehouse Rd, Suite 500 East,  
P.O. Box 747, Falls Church, VA, 22040-0747, US  
CLMN Number of Claims: 21  
ECL Exemplary Claim: 1  
DRWN 1 Drawing Page(s)  
LN CNT #46  
CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
AB A family of structurally rigid dopamine D3 receptor selective ligands is  
described. The family of structurally rigid dopamine D3 receptor  
selective ligands has the formula wherein A is cis or trans  
--CH.dbd.CH--, --C.dbd.C--, or cyclohexyl. B is cis or trans  
--CH.dbd.CH-- or absent. R1 represents an optionally substituted phenyl  
group, wherein said substituents are selected from the group consisting  
of: hydrogen, halogen, amino, nitro, hydroxyl, alkoxy, alkyl, acyl and  
pyridyl, and said substitution may occur at any of the ortho, meta, or  
para positions, or R1 represents a heteroaromatic ring. A preferred  
heteroaromatic ring is indole, quinoxaline, pyridyl, pyrimidyl, or  
imidazole. R2 and R3 may be independently hydrogen or a halogen, or R2  
alone may be Cl, C2, or C3 alkoxy, and m is 1 or 2, and n is 0, 1, or 2.  
CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
IT 675599-27-6P 675599-28-7P  
(preparation of structurally rigid arylpiperazines as dopamine D3 receptor  
selective ligands)  
IT 675599-29-8 675599-30-1 675599-31-2  
675599-32-3 675599-34-5 675599-35-6  
675599-36-7 675599-38-9 675599-39-0  
675599-41-4 675599-43-6 675599-45-8  
675599-46-9 675599-47-0 675599-48-1  
675599-49-2 675599-51-6 675599-52-7  
675599-53-8 675599-54-9 675599-55-0  
675599-56-1 675599-58-3 675599-59-4  
675599-61-8 675599-62-9 675599-64-1  
675599-65-2 675599-66-3 675599-67-4  
675599-68-5 675599-69-6 675599-71-0  
675599-72-1 675599-73-2 675599-74-3  
(preparation of structurally rigid arylpiperazines as dopamine D3 receptor  
selective ligands)  
IT 675599-27-6P  
(preparation of structurally rigid arylpiperazines as dopamine D3 receptor  
selective ligands)  
RN 675599-27-6 USPATFULL  
CN Benamide, N-[(2E)-4-[4-[(2,3-dichlorophenyl)-1-piperazinyl]-2-butenyl]-4-  
iodo-, ethanedicarboxylate (SCI) (CA INDEX NAME)  
CM 1  
CRN 675599-26-5  
CMF C21 H22 Cl2 I N3 O  
Double bond geometry as shown.

L42 ANSWER 1 OF 3 USPATFULL on STN (Continued)



CM 2

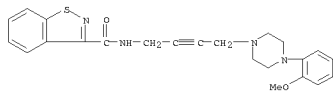
CRN 144-62-7

CMF C2 H2 O4



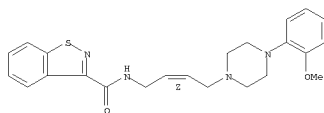
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L42 ANSWER 2 OF 3 USPATFULL on SIN  
 AN 92:54726 USPATFULL  
 TI Benzisothiazole- and benzisoxazole-3-carboxamides  
 IN Hrib, Nicholas J., Somerville, NJ, United States  
 Jurcak, John G., Union City, NJ, United States  
 PA Hoechst-Roussel Pharmaceuticals Incorporated, Somerville, NJ, United States (U.S. corporation)  
 PI US-----5225412 19930706  
 AI 1992US-000899518 19920616 (7)  
 RLI Division of Ser. No. 1991US-000693168, filed on 29 Apr 1991, now patented, Pat. No. US-----5143923  
 DT Utility  
 FS Granted  
 EXNAM Primary Examiner: Tsang, Cecilia  
 LREP Wittekind, Raymond R.  
 CLMN Number of Claims: 31  
 ECL Exemplary Claim: 1,24,26  
 DRWN No Drawings  
 LN.CNT 1189  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 AB Novel benzisothiazole- and benzisoxazole-3-carboxamides, processes and intermediates for the preparation thereof, and methods of treating psychoses utilizing compounds and compositions thereof are disclosed.  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 IT 145759-36-0P 145759-37-1P  
 (preparation of, as antipsychotic)  
 RN 145759-36-0 USPATFULL  
 CN 1,2-Benzisothiazole-3-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]-2-butenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



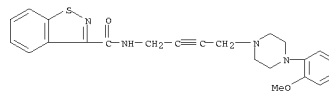
●2 HCl

RN 145759-37-1 USPATFULL  
 CN 1,2-Benzisothiazole-3-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]-2-butenyl]-, dihydrochloride, (Z)- (9CI) (CA INDEX NAME)  
 Double bond geometry as shown.



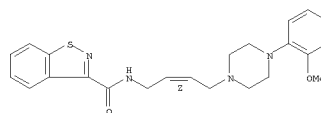
●2 HCl

L42 ANSWER 3 OF 3 USPATFULL on SIN  
 AN 92:72477 USPATFULL  
 TI Benzisothiazole- and benzisoxazole-3-carboxamides  
 IN Hrib, Nicholas J., Somerville, NJ, United States  
 Jurcak, John G., Union City, NJ, United States  
 PA Hoechst-Roussel Pharmaceuticals Inc., Somerville, NJ, United States (U.S. corporation)  
 PI US-----5143923 19920901  
 AI 1991US-000693168 19910429 (7)  
 DT Utility  
 FS Granted  
 EXNAM Primary Examiner: Tsang, Cecilia  
 LREP Wittekind, Raymond R.  
 CLMN Number of Claims: 21  
 ECL Exemplary Claim: 1  
 DRWN No Drawings  
 LN.CNT 1158  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 AB Novel benzisothiazole- and benzisoxazole-3-carboxamides, processes and intermediates for the preparation thereof, and methods of treating psychoses utilizing compounds and compositions thereof are disclosed.  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 IT 145759-36-0P 145759-37-1P  
 (preparation of, as antipsychotic)  
 RN 145759-36-0 USPATFULL  
 CN 1,2-Benzisothiazole-3-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]-2-butenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 145759-37-1 USPATFULL  
 CN 1,2-Benzisothiazole-3-carboxamide, N-[4-[4-(2-methoxyphenyl)-1-piperazinyl]-2-butenyl]-, dihydrochloride, (Z)- (9CI) (CA INDEX NAME)  
 Double bond geometry as shown.



●2 HCl

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(FILE 'HOME' ENTERED AT 10:36:06 ON 04 APR 2008)

FILE 'HCAPLUS' ENTERED AT 10:36:17 ON 04 APR 2008

L1 1 US5143923/PN

FILE 'REGISTRY' ENTERED AT 10:36:32 ON 04 APR 2008

FILE 'HCAPLUS' ENTERED AT 10:36:32 ON 04 APR 2008

L2 TRA L1 1- RN : 79 TERMS

FILE 'REGISTRY' ENTERED AT 10:36:32 ON 04 APR 2008

L3 79 SEA L2

L4 32 L3 AND NC2NC2/ES

L5 18 L4 AND NSC3-C6/ES

FILE 'HCAPLUS' ENTERED AT 11:19:51 ON 04 APR 2008

L6 1 US20060106030/PN

FILE 'REGISTRY' ENTERED AT 11:20:04 ON 04 APR 2008

FILE 'HCAPLUS' ENTERED AT 11:20:04 ON 04 APR 2008

L7 TRA L6 1- RN : 46 TERMS

FILE 'REGISTRY' ENTERED AT 11:20:04 ON 04 APR 2008

L8 46 SEA L7

L9 41 L8 AND NC2NC2/ES AND 46.150.18/RID

L10 14 L9 AND (NC5 OR NC2NC2-C6 OR OC4-C6 OR SC4-C6 OR C5-C6-C6)/ES

L11 STR

L12 12 L11

L13 SCR 1011 OR 1012 OR 1013 OR 1019

L14 46 L11 AND L13

L15 SCR 1840

L16 46 L11 AND L13 AND L15

L17 17940 L11 AND L13 AND L15 FULL

SAV TEM J594C1GVI/A L17

L18 STR L11

L19 50 L13 SAM SUB=L17

L20 STR L18

L21 50 L20 SAM SUB=L17

L22 38 L17 AND L8

L23 8285 L20 FULL SUB=L17

L24 9655 L17 NOT L23

L25 STR L11

L26 STR L25

L27 1 (L25 OR L26) SAM SUB=L24

L28 1 L26 SAM SUB=L24

L29 0 L25 SAM SUB=L24

L30 13 (L25 OR L26) FULL SUB=L24

L31 3 L30 AND L8

FILE 'HCAPLUS' ENTERED AT 12:55:10 ON 04 APR 2008

L32 3 L30

L33 2 L22

FILE 'REGISTRY' ENTERED AT 12:59:51 ON 04 APR 2008

L34 110 C23H24CL2N4O

L35 0 L34 AND L17

L36 22 L34 AND NC2NC2/ES

L37 0 L36 AND NC4-C6/ES

FILE 'HCAOLD' ENTERED AT 13:01:10 ON 04 APR 2008

L38 0 L22

L39 0 L30

FILE 'USPATFULL, USPATOLD, USPAT2' ENTERED AT 13:01:53 ON 04 APR 2008

L40 1 L22

L41 3 L30

L42            3 L40-41

FILE 'HCAPLUS' ENTERED AT 13:03:22 ON 04 APR 2008

L43            1 L32 AND L33

L44            2 L32 NOT L43

L45            2 L33,L43

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